

Getting Started with the NCCS

NCCS USERS MEETING



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Outline

- **Computational resources**
- **Support options**
- **Common features**
- **Managing your allocations**

- **X1E overview**
- **XT4 overview**

Jaguar - Cray XT4

- 11,708 Nodes
- 2.6Ghz dual core AMD Opteron
 - Compute nodes
 - Service nodes
- 119TF
- 46TB Main Memory
- 600TB Local Disk
- Lustre filesystem
- Unicos/lc
 - Linux/Catamount
- 250TF coming. . .



Phoenix - Cray X1E

- 1024 Multi Streaming Processors (MSP)
- 2TB Memory
- 18.5TF
- Largest X1E
- Linux cross compiler
 - robin.ccs.ornl.gov
 - robin1.ccs.ornl.gov



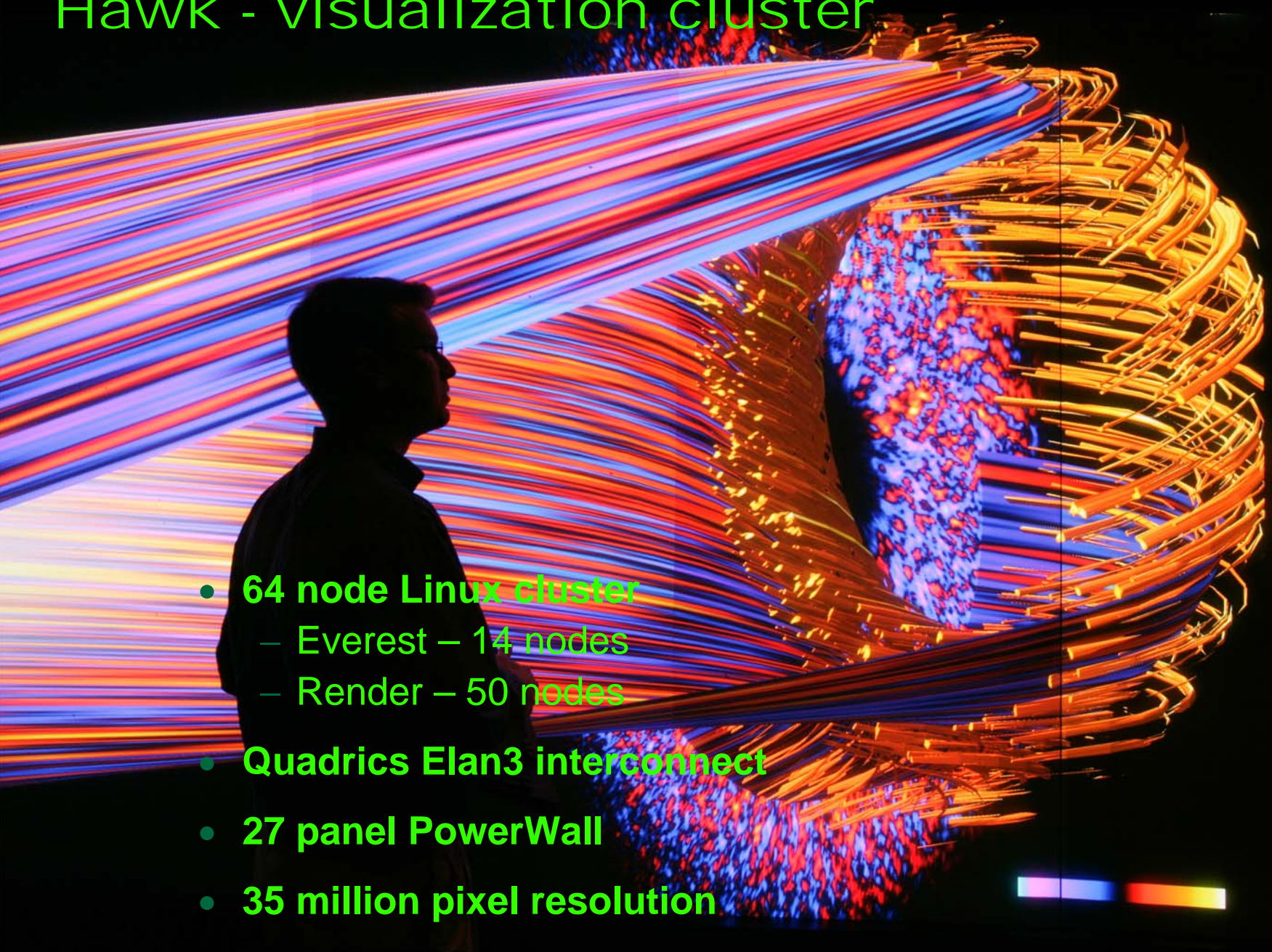
Ram - SGI Altix

- 2x Intel Itanium2 processors
- 2TB shared memory
- Resource for pre/post processing of data



Hawk - visualization cluster

- **64 node Linux cluster**
 - Everest – 14 nodes
 - Render – 50 nodes
- **Quadrics Elan3 interconnect**
- **27 panel PowerWall**
- **35 million pixel resolution**



HPSS – Mass Storage

- Tape library and disk storage
 - 6 second access time
- Suitable for backup and long term storage
- 1.3PB stored data
- Expandable to 5PB
- hsi to access
 - FTP-like interface



How to get help:

- **Web (www.nccs.gov)**
 - System status
 - FAQs
 - Available software
- **Email (help@nccs.gov)**
 - User Assistance Center
 - M-F 9am-5pm ET
- **Phone (865-241-6536)**
 - 24/7

System Status



Jaguar Phoenix Ram



Hawk



HPSS

Contact the NCCS User
Assistance Center

Web support

- System Status
- Resource Info
- Available software

NATIONAL CENTER FOR COMPUTATIONAL SCIENCES

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The National Center for Computational Sciences (NCCS) at the Oak Ridge National Laboratory was established in 1992 and in 2004 was designated by the Secretary of Energy as the Leadership Computing Facility for the nation, to provide for unclassified research a resource 100 times more powerful than current capabilities.

The facility provides researchers an unparalleled environment for new discoveries that will dramatically impact the nation's ability to produce a secure energy economy and increase mankind's understanding of our world. As a designated User Facility, the NCCS will Deliver leadership-class computing for science and engineering

- Focus on grand challenge science and engineering applications
- Procure largest-scale computer systems (beyond vendor design point) and develop high-end operational and application software

Highlights

The First NCCS Users Meeting will be held February 14-16. [Register now!](#)

DOE's Office of Science Awards 18 Million Hours of Supercomputing Time to 15 Teams for Large-Scale Scientific Computing

2006 DOE INCITE Supercomputing Allocations

Doug Kothe Named Director of Science for NCCS

Cray, ORNL are a Winning Team

System Status

↑ ↑ ↑
Jaguar Phoenix Ram

↑ ↑
Hawk HPSS

Contact the NCCS User Assistance Center

Phoenix



Jaguar



- Open Issues
- C/C++
- Fortran
- File Systems
- Batch Jobs
- Interactive
- System Stat
- FAQ
- Cray Perform

- Open Issues
- C/C++
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- File Systems
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- System Status

Phoenix is a Cray X1E provided as a primary system in the National Center for Computational Sciences (NCCS).

Jaguar is a Cray XT3 provided as a primary system in the National Leadership Computing Facility (NLCF).

The current Jaguar installation has 5294 nodes, each with a 2.4-GHz AMD Opteron processor and 2 GB of memory. 5212 nodes are available in the compute partition, and the remainder provide I/O and login services.

Each node is connected to a Cray Seastar router through Hypertransport, and the Seastars are all interconnected in a 3D-torus topology. The resulting interconnect has very high bandwidth, low latency, and extreme scalability.

The operating system is UNICOS/lc, which is a combination of Linux on the service nodes and the Catamount microkernel on the compute nodes. Catamount is designed to minimize system overhead, thus allowing scalable low-latency global communication.

External Links:

- Cray XT3 Overview at Cray, Inc.
- Red Storm, the project between Cray and Sandia National Laboratories that led to the XT3 product.

Libraries

		version	jaguar	phoenix	ram	hawk
ATLAS						
AZTEC	CDAT	4.0b4			x	
BLACS	Cg	1.4.0-4				x
BLAS	Ensign	7.6.4			x	
FFTPa	GAMESS	jan2004			x	
FFTW	gdb	5.0		x		
		5.3.90	x			
Global		6.1			x	
		version	jaguar	phoenix	ram	hawk
	gmake	3.7.9		x	x	
HDF5		3.8.0	x			
	Grace	4.1.18			x	
	Histx	1.2a			x	
	Ncarg	4.3.1			x	
		4.4.1		x		



Email support

- **help@nccs.gov**

- **RT system**

- Automated response

- **Help us help you**

- Username
- Description
- Machine
- Error messages

- **Distribution Lists**

Jaguar: <https://email.ornl.gov/mailman/listinfo/jaguar-notice>

Phoenix: <https://email.ornl.gov/mailman/listinfo/phoenix-notice>

Dear NCCS User,

This is an automated response to your NCCS support inquiry. You have been assigned ticket #14516. If you wish to add more information to this ticket, simply reply to this message without modifying the subject line. To report a separate issue, email help@nccs.gov with a new subject line.

For the fastest possible response, make sure your ticket includes the machine name, the system name(s) and the location of any executables, scripts, or output files related to the error. For batch jobs, please include the job ID number.

Information including scheduled outages, system availability, and current system issues can be found at <http://info.nccs.gov>.

The NCCS User Assistance Center is staffed Monday through Friday, 9:00 AM to 5:00 PM Eastern Time.

NCCS User Assistance Center

Phone support

- **24/7 phone support**
- **Staffed daily**
 - M-F 9am-5pm ET
- **865-241-6536**
- **Monthly teleconference**
 - All NCCS users invited



Common features

- **NFS shared home directory**
 - 500MB quota
- **Scratch space**
 - Temporary storage on lustre filesystem
 - /tmp/work/<username>
 - Daily sweep for files >7 days old
- **Access to HPSS**
- **One time password access**
- **Totalview debugger**
- **Modules**

Connecting

- **Use Secure Shell**

- `ssh userid@<machine>.ccs.ornl.gov`
- `ssh bob@phoenix.ccs.ornl.gov`

- **One time password**

- RSA SecurID
- PASSCODE = PIN + Token Code
- SSH client need keyboard-interactive



RSA SecurID®

Modules

- **Consistent environment setup**
- **Commands**
 - module list
 - module avail
 - module load <module>
 - module unload <module>
 - module swap <old> <new>
 - module purge
 - module help
- **Examples**
 - module load subversion
 - module load modules (man pages for module)

Tips

- **Home directory quota 500MB**
 - Use scratch space - /tmp/work/<user>
- **Use *lsquota* to determine disk quota**
- **HPSS works best with >1GB files**
 - tar cvf - . | hsi put - : data.tar
- **Need software installed?**
 - module load avail
 - help@nccs.gov

Accounting

- **Every project has an identifier**
 - FUSXXX, CHMYYYzzz, etc
- **Include in PBS scripts**
 - #PBS -A FUS123
- **No identifier = no submission**
- **Aids in proper accounting of allocations**

Managing Allocations

- **Adding access or users**
 - <https://secure.ccs.ornl.gov/request.new.html>
- **Subprojects**
 - Available by request
- **Project web space available**
 - users.nccs.gov/<projectID>
- **Allocation usage**
 - Available on project pages
 - command line - %> showusage

Special Requests

- **Exceptions to NCCS policies are possible**
- **Relaxed Queue Limits**
 - Need to run a job longer than normal queue limits?
- **System Reservation**
 - Need dedicated access for important jobs?
- **Disk Quota Increase**
- **Scratch Purge Exemption**
- ☐ <http://info.nccs.gov/resources/general/specialrequests>

How can we help you?

- **Suggestions encouraged**

- help@nccs.gov
- <https://info.nccs.gov/forms/specialrequest/suggestion.php>